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TEMPERATURE DEPENDENCE OF ELASTIC MODULI FOR NACL

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ABSTRACT

In earlier studies sound velocities and elastic moduli of some minerals like MgO, $MgAl_2O_4$, Al_2O_3, $Y_3Al_2(AlO_4)_3$ and pyrope ($Mg_3Al_2Si_3O_{12}$) up to a pressure of 200 GPa have been analyzed. The Hama-Suito theory of equation of state based on the Augmented Plane Wave (APW) and quantum statistical methods have been used for the determination of pressure-density relationships. In present work, Holzapfel AP2 equation of state is being used for calculating the elastic moduli such as shear modulus, Young's modulus and Poisson's ratio as a function of pressure for NaCl. Results thus obtained are furnished and found to be in close agreement with the available experimental data.

KEYWORDS: Shear Modulus, Young's Modulus, Poisson's Ratio & Equation of State

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INTRODUCTION

Experimental values of sound velocities for minerals are determined by measuring slopes of dispersion curves near the Brilliouin zone center, i.e. d ω/dk, where ω is the mode frequency and k is the wave vector related to lattice constant a by k = 2π/a (Refs 1-4). There are mainly two types of sound velocities V_p for compressional or longitudinal waves and V_s for shear or transverse waves. The dependence of longitudinal and transverse wave velocities on elastic moduli i.e. bulk modulus (K), shear modulus (G) and density (ρ) is given by following relation[1,5].

$$V_P = \left[\frac{K+\frac{4}{3}G}{\rho}\right]^{1/2} \tag{1}$$

$$V_S = \left[\frac{G}{\rho}\right]^{1/2} \tag{2}$$

Chopelas *et al.*[1] in his work measured the experimental values of sound velocities for five minerals using the side band fluore scence method[3,6,7] up to pressures corresponding to the mantle region of the earth. These minerals are MgO, $MgAl_2O_4$, Al_2O_3, $Y_3Al_2(AlO_4)_3$ and pyrope ($Mg_3Al_2Si_3O_{12}$). The pressure derivatives of the bulk modulus and shear modulus have also been reported[1], which present the good agreement with the lower pressure values based on ultrasonic measurement.

In the present study, a method has been developed for calculating the theoretical values of shear modulus, Young's modulus and Poisson's ratio for NaCl using Holzapfel AP2 equation of state. The results are found to be in close agreement with the experimental values.

Original Article

Theory

The isotropic shear modulus (G) within the Voigt limit[5] is as follows:

$$G = \frac{1}{5}(2C_s + 3C_{44}) \tag{3}$$

$$\text{Where } C_s = \frac{1}{2}(C_{11} - C_{12}) \tag{4}$$

The adiabatic bulk modulus for cubic solid is:

$$K = \frac{(C_{11}+2C_{12})}{3} \tag{5}$$

The Cauchy relation for elastic constants is:

$$C_{12} - C_{44} = 2P \tag{6}$$

Using equations (3) to (6), we find:

$$G = \frac{3}{5}(K - 2P) \tag{7}$$

Using equation (7), we can write the first pressure derivative of shear modulus dG/dP as:

$$G' = \frac{3}{5}(K' - 2) \tag{8}$$

According to static and dynamic elasticity, Young's modulus (Y) is related compressional and shear velocities as follows:

$$Y = \rho V_S \left[\frac{4{V_S}^2 - 3{V_P}^2}{{V_S}^2 - 4{V_P}^2}\right] \tag{9}$$

We can rewrite Equation (9) in the terms of bulk and shear modulus with the help of equations (1) and (2) as follows:

$$Y = \frac{9KG}{3K+G} \tag{10}$$

The Poisson's ratio is determined by the following formula[5]:

$$\sigma = \frac{3K+4P}{12K-4P} \tag{11}$$

We make use of equations (7) - (11) for calculating shear modulus, its pressure derivative, Young's modulus and Poisson's ratio with the help of K and P as a function of density. The pressure-density relationships and bulk modulus can be obtained with the help of an equation of state.

The Holzapfel AP2 EOS can be written as[9,10]:

$$P = 3\,K_0\,x^{-5}\,(1-x)\,[1 + c_2 x(1-x)\,]\,\exp[c_0\,(1- x)] \tag{12}$$

$$\text{Where, } x = \left[\frac{V}{V_0}\right]^{1/3} \text{ and } c_0 = -\ln\left(\frac{K_0}{P_{FGO}}\right) \tag{13}$$

$$P_{FGO} = a_{FG}\left(\frac{Z}{V_0}\right)^{5/3} \tag{14}$$

With $a_{FG} = 0.02337$ GPa nm[11]. Z is the total number of electrons in the Volume V_0. In the case of NaCl, we have Z=28 per molecule. This is to be multiplied by the Avogadro number when V_0 is given in the units of cm3/mole. The constant c_2 in Equation (12) is related to K'_0, The value of $K' = \frac{dK}{dP}$, at P = 0, as follows:

$$C_2 = \frac{3}{2}\left(K'_0 - 3\right) - C_0 \tag{15}$$

P-V relationships along different isotherms for NaCl, have been determined by using Equation(12). The required input data for V0, K0, and K'0 at different temperatures have been taken from the literature[12,13,14,15] (Table 1). The V0lume ratio V/V0 in the table represents V(T,P)/V(T,0) along different isotherms at selected temperatures T. The amount of pressure required to produce the same change in V/V0 decreases continuously with the increase in temperature. This is related to the fact that the bulk modulus becomes less and the material becomes more compressible at higher temperatures.

Table 1: Values of Input Parameters for NaCl 12, 13, 14
Used in the Holzapfel AP2 EOS

T(K)	V_0=V(T,0) (cm3/mol)	Ko (GPa)	K'_0	P_{FG0} (GPa)	C_0	C_2
300	27.015	24.0	5.35	1065.62	2.70	0.83
450	27.523	21.6	5.51	1033.05	2.77	0.99
600	28.101	19.0	5.73	997.87	2.87	1.22
750	28.757	16.5	6.03	960.19	2.97	1.58
900	29.517	14.1	6.40	919.39	3.08	2.02
1050	30.419	11.7	6.85	874.39	3.22	2.57

In addition to P-V isotherms, the high derivative properties along different isotherms can also be calculated using values of input parameters appropriately corresponding to each temperature. This method has successfully been used by earlier researchers[13, 14, 16]. The expressions for the bulk modulus K and its pressure derivatives K'=dK/dP and $K''=d^2K/dP^2$ is obtained using the following relationships:

$$K = -\left(\frac{dP}{dV}\right) = -\frac{x}{3}\left(\frac{dP}{dx}\right) \tag{16}$$

$$K' = -\frac{x}{3} \tag{17}$$

$$KK'' = \frac{x^2}{9K}\left(\frac{d^2K}{dx^2}\right) - K'\left(K' + \frac{1}{3}\right) \tag{18}$$

Where,

$$\frac{dK}{dx} = -\frac{x}{3}\left(\frac{d^2P}{dx^2}\right) - \frac{1}{3}\left(\frac{dP}{dx}\right) \tag{19}$$

$$\text{And } \frac{d^2K}{dx^2} = -\frac{x}{3}\left(\frac{d^3P}{dx^3}\right) - \frac{2}{3}\left(\frac{d^2P}{dx^2}\right) \tag{20}$$

The pressure P as a function of x is given by Equation (12), the Holzapfel AP2 EOS.

RESULTS AND DISCUSSIONS

Using Holzapfel AP2 EOS, elastic moduli i.e. shear modulus, Young's modulus, and Poisson's ratio has been calculated for NaCl and the calculated values have been tabulated in table2. The calculated values are in close agreement with the standard results[17].

Table 2: Output Elastic Moduli of Nacl at Different Temperatures

T(K)	V/V_O	P (GP_a)	K (GP_a)	G (GP_a)	Y(GP_a)	σ
300	1	0	24	14.40	36	0.25
450	0.95	1.28	28.3	15.44	39.19	0.269
600	0.90	2.69	33	16.57	42.58	0.284
750	0.85	4.32	38.9	18.15	47.12	0.298
900	0.80	6.22	46.1	20.19	52.85	0.308
1050	0.75	8.45	54.7	22.68	59.78	0.317

With the help of table 2, the graphs between temperature and shear modulus, Young's modulus and Poisson's ratio have been plotted for NaCl upto 1050K. The variation of elastic moduli is shown in figure 1, figure 2 and figure 3 it has been observed that shear modulus, Young's modulus and Poisson's ratio increases with increase in temperature.

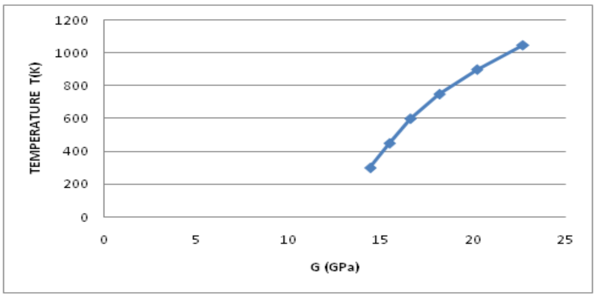

Figure 1: Variation of Shear Modulus with Temperature

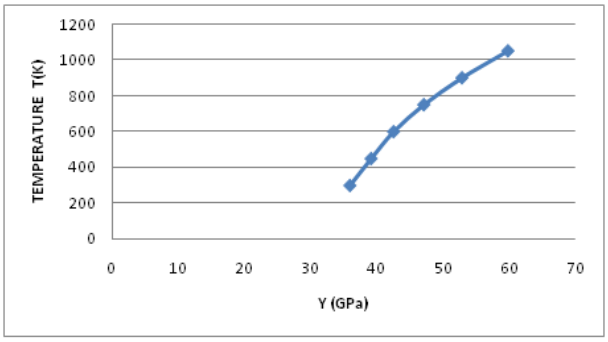

Figure 2: **Variation of Young's Modulus with Temperature**

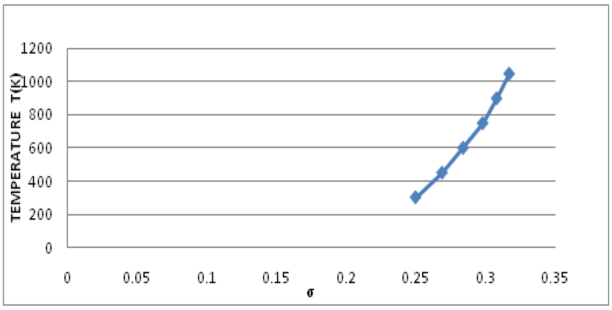

Figure 3: **Variation of Poisson's Ratio with Temperature**

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